Supporting Information

Electron Transfer Processes in Metal-Free Tetraferrocenylporphyrin. Understanding Internal Interactions to Access Mixed-Valence States Potentially Useful for Quantum Cellular Automata

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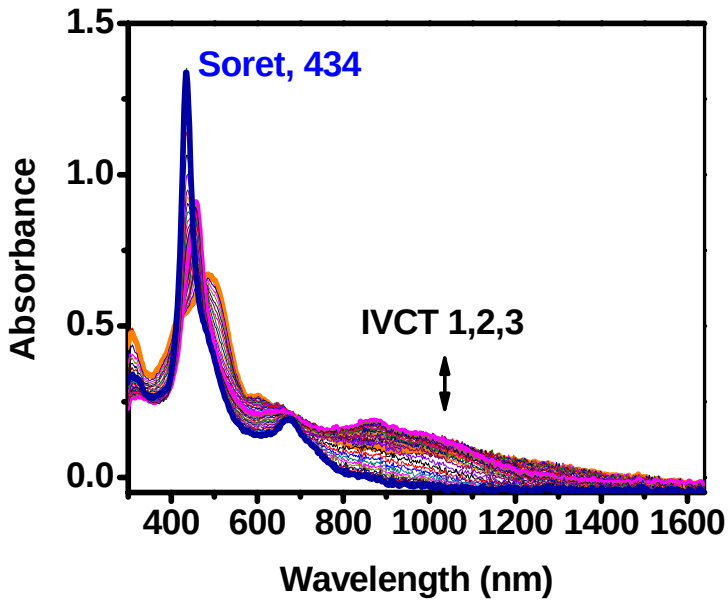
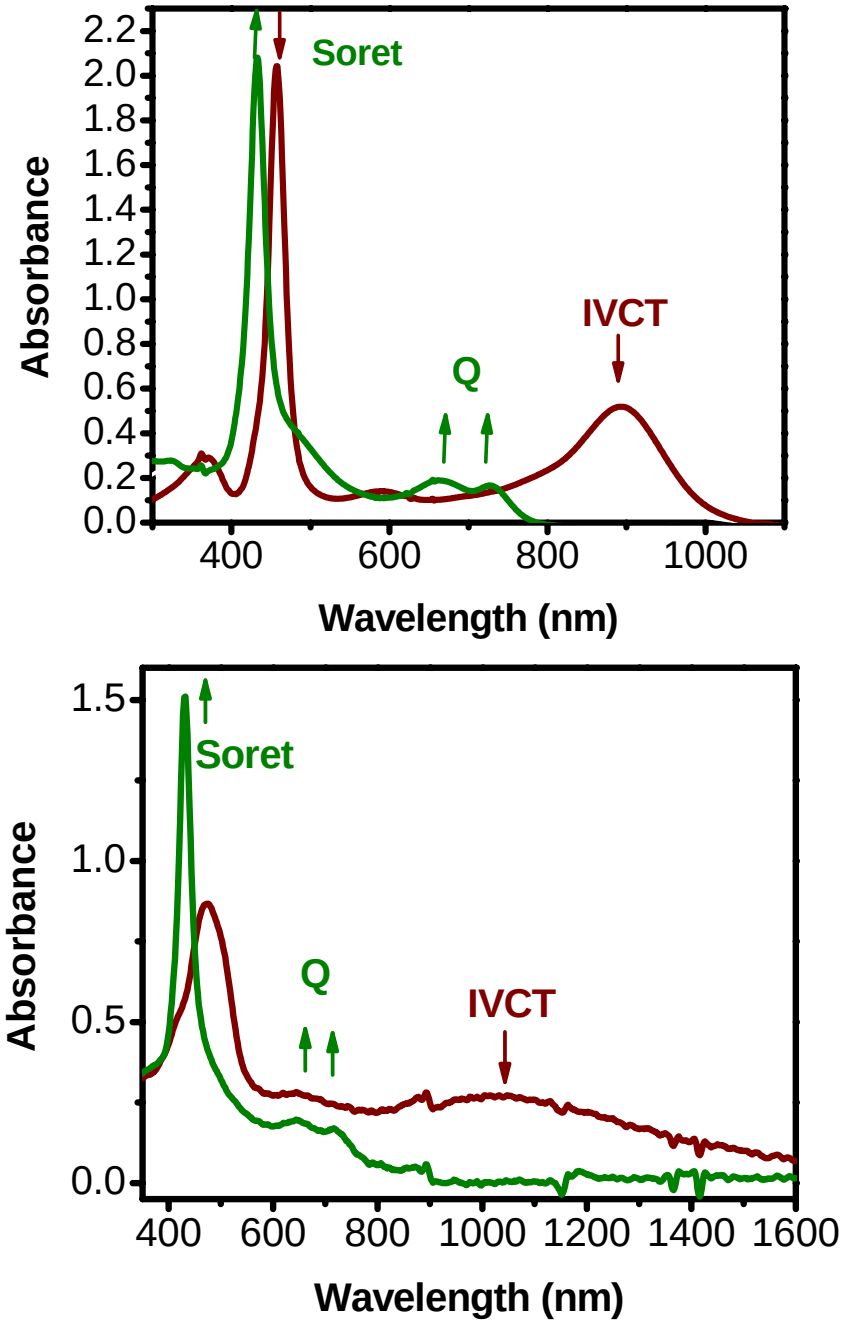
Full citation for Gaussian 03:

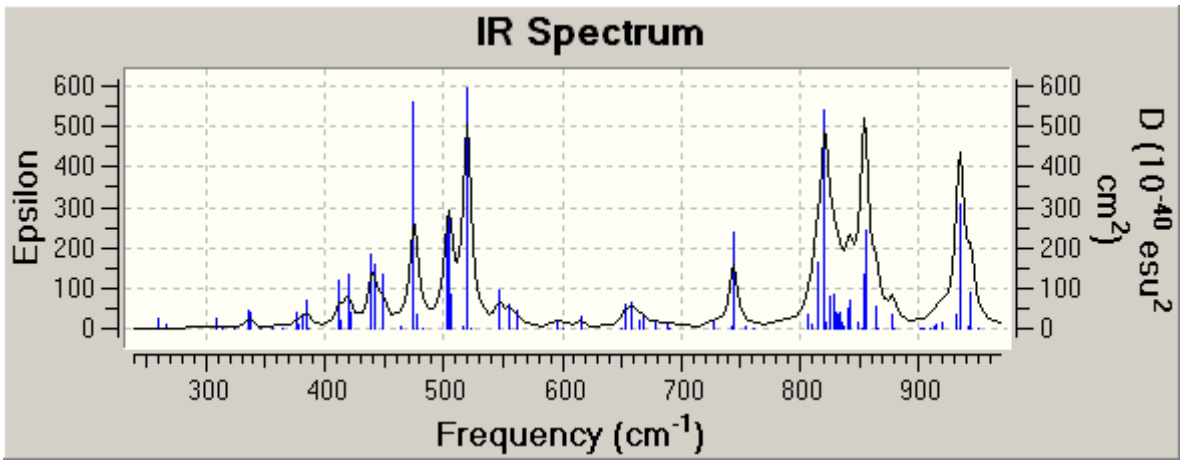
[37] M. J. Frisch, G.W. Trucks, H. B. Schlegel, G. E. Scuseria,M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J.M.Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov,G. Liu,A. Liashenko, P. Piskorz, I. Komaromi, R. L.Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara,M. Challacombe, P.M.W. Gill, B. G. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *GAUSSIAN 03 (Revision C.02)*, Gaussian, Inc., Wallingford, CT, 2004.



Supporting Information Figure 1. Spectroelectrochemical formation of neutral H_2TFcP from oxidized forms.

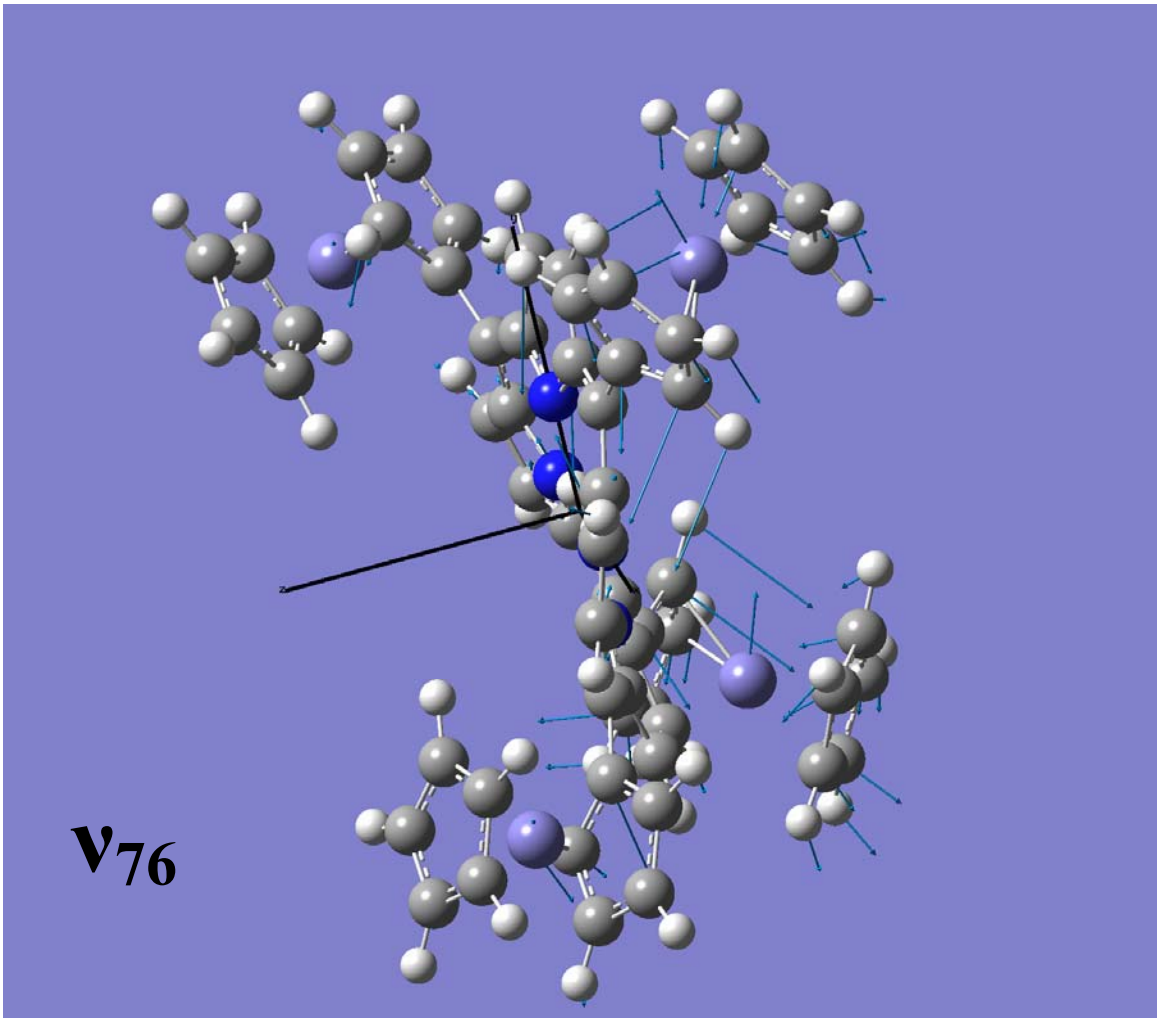


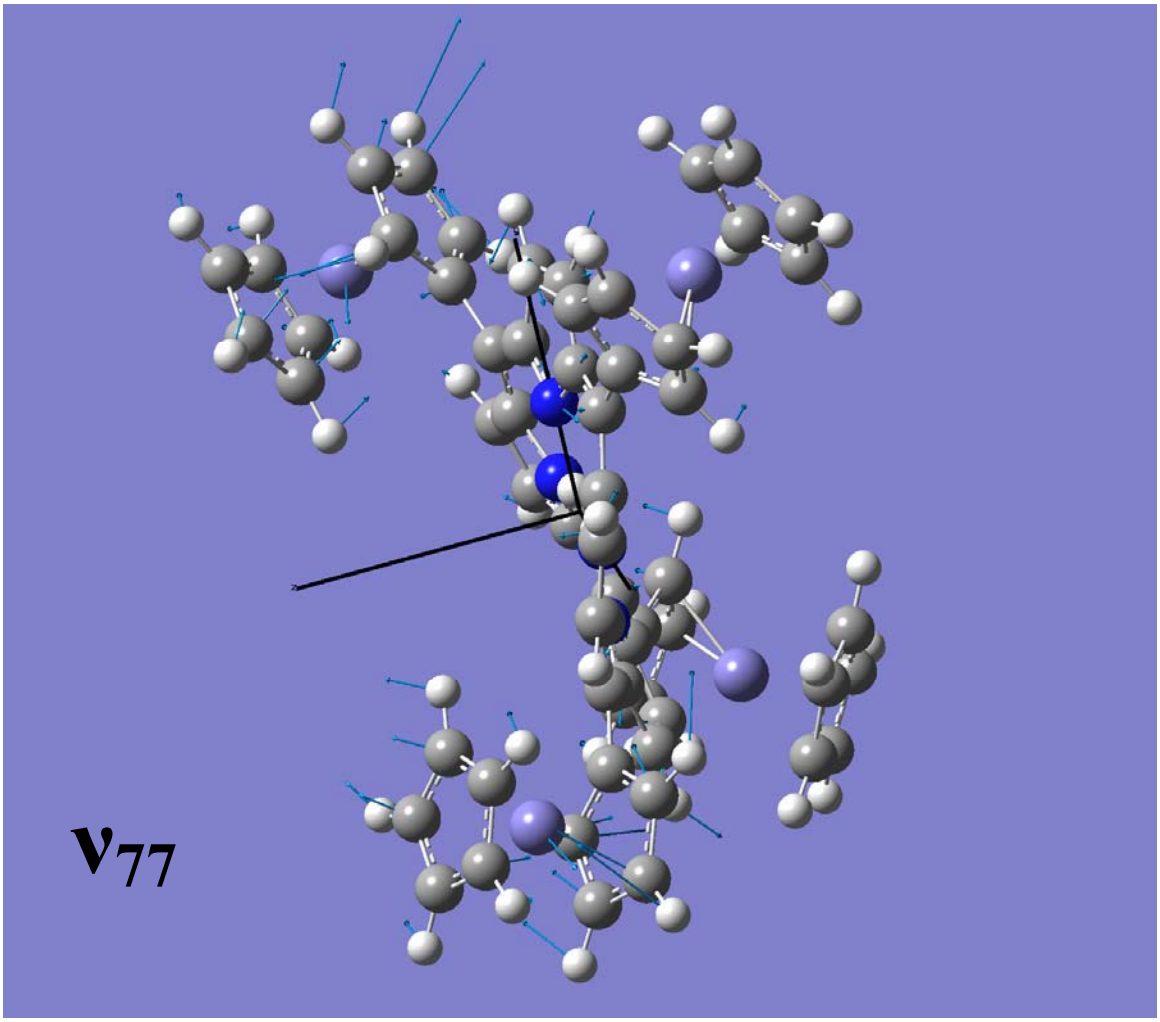
Supporting Information Figure 2. Formation of the neutral H_2TFcP from $[H_2TFcP]^{+}$ (top) and $[H_2TFcP]^{3+}$ (bottom).



Supporting Information Figure 3. IR spectrum of H_2TFcP predicted by DFT at B3LYP/6-31G(d) level.

Supporting Information Figure 4. IR displacement vectors of selected vibrational modes (76,77,11,113,115,116,136-140,170,171,174,175) of H_2TFcP predicted by DFT at the B3LYP/6-31G(d) level

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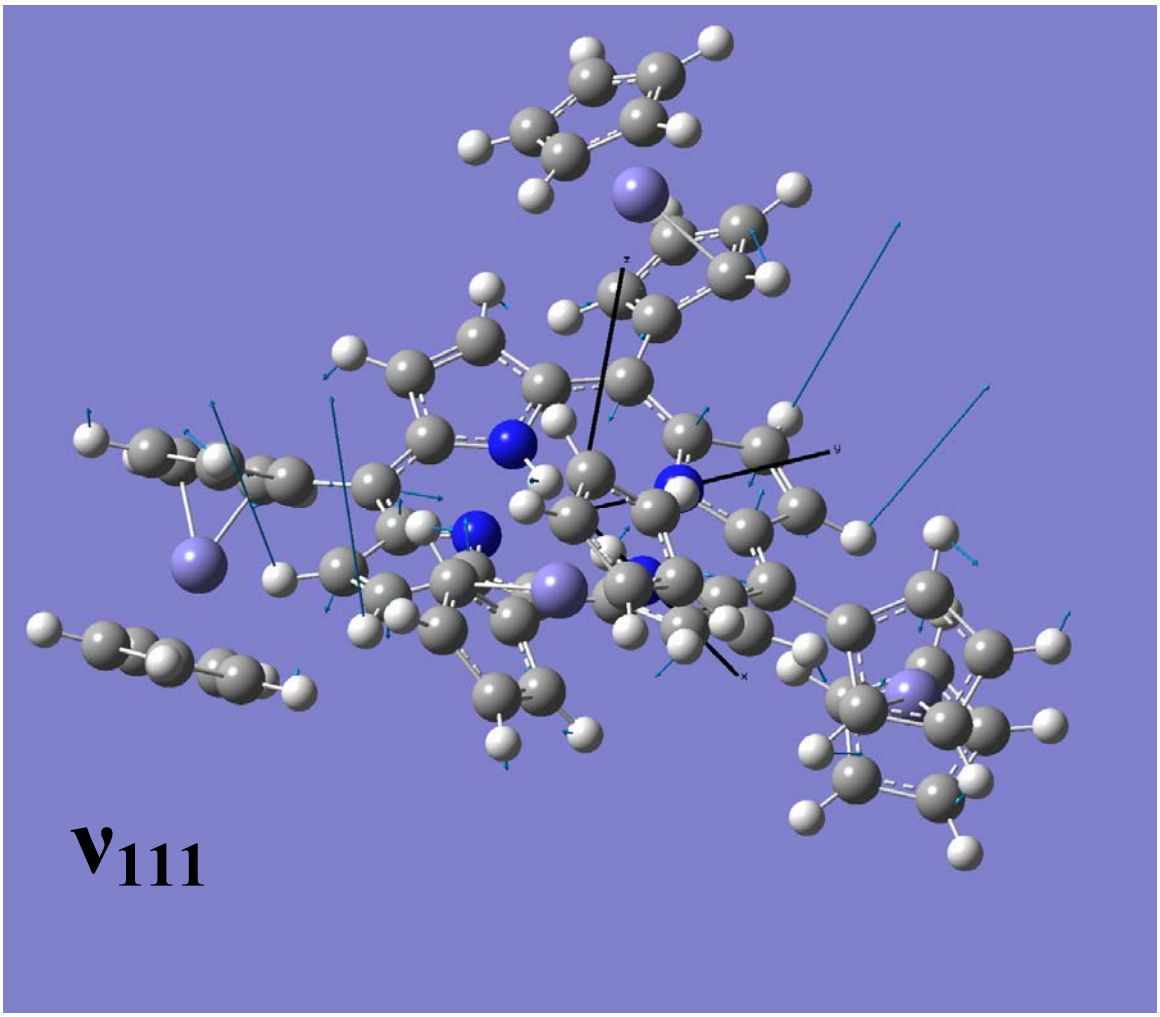
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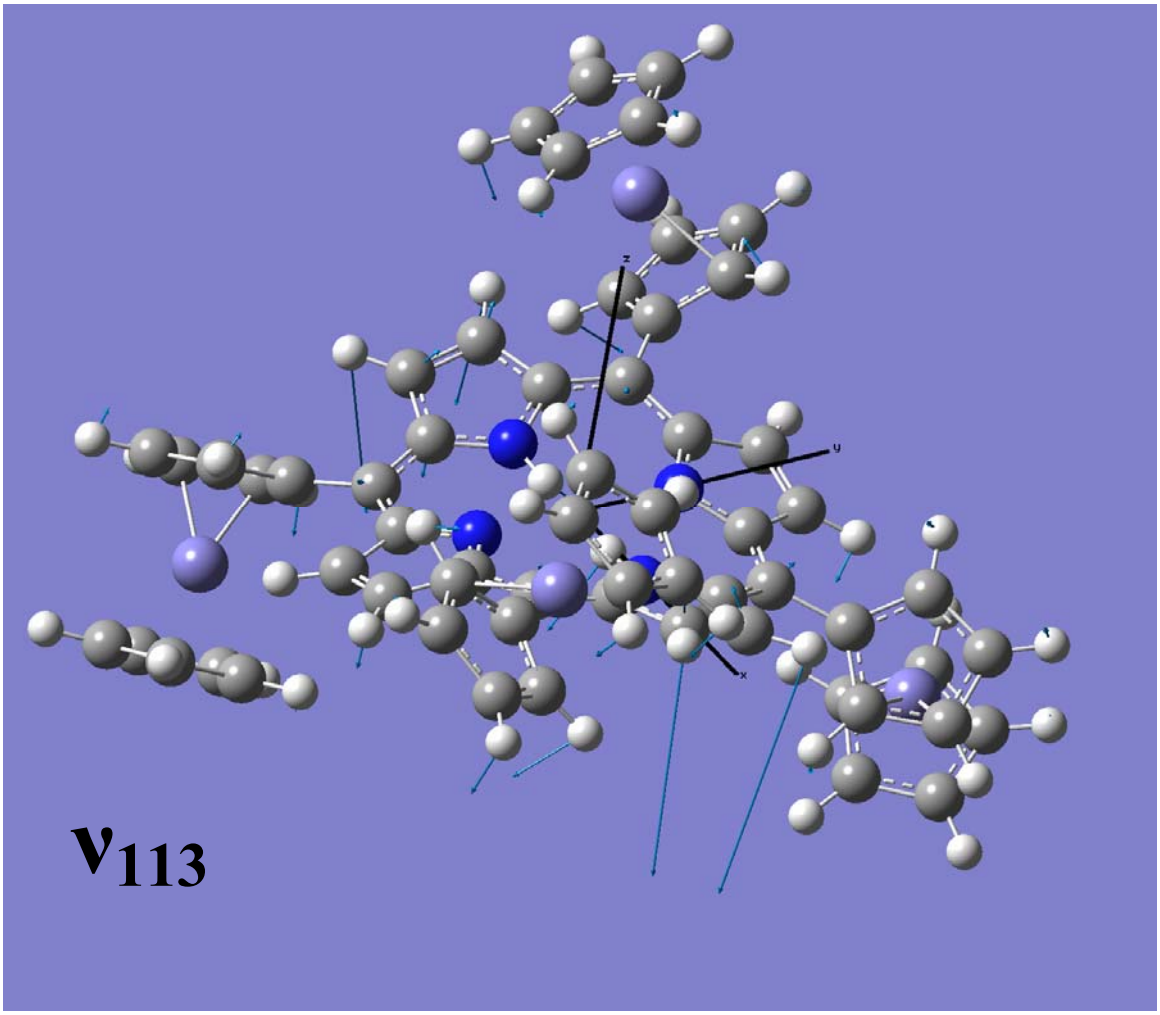
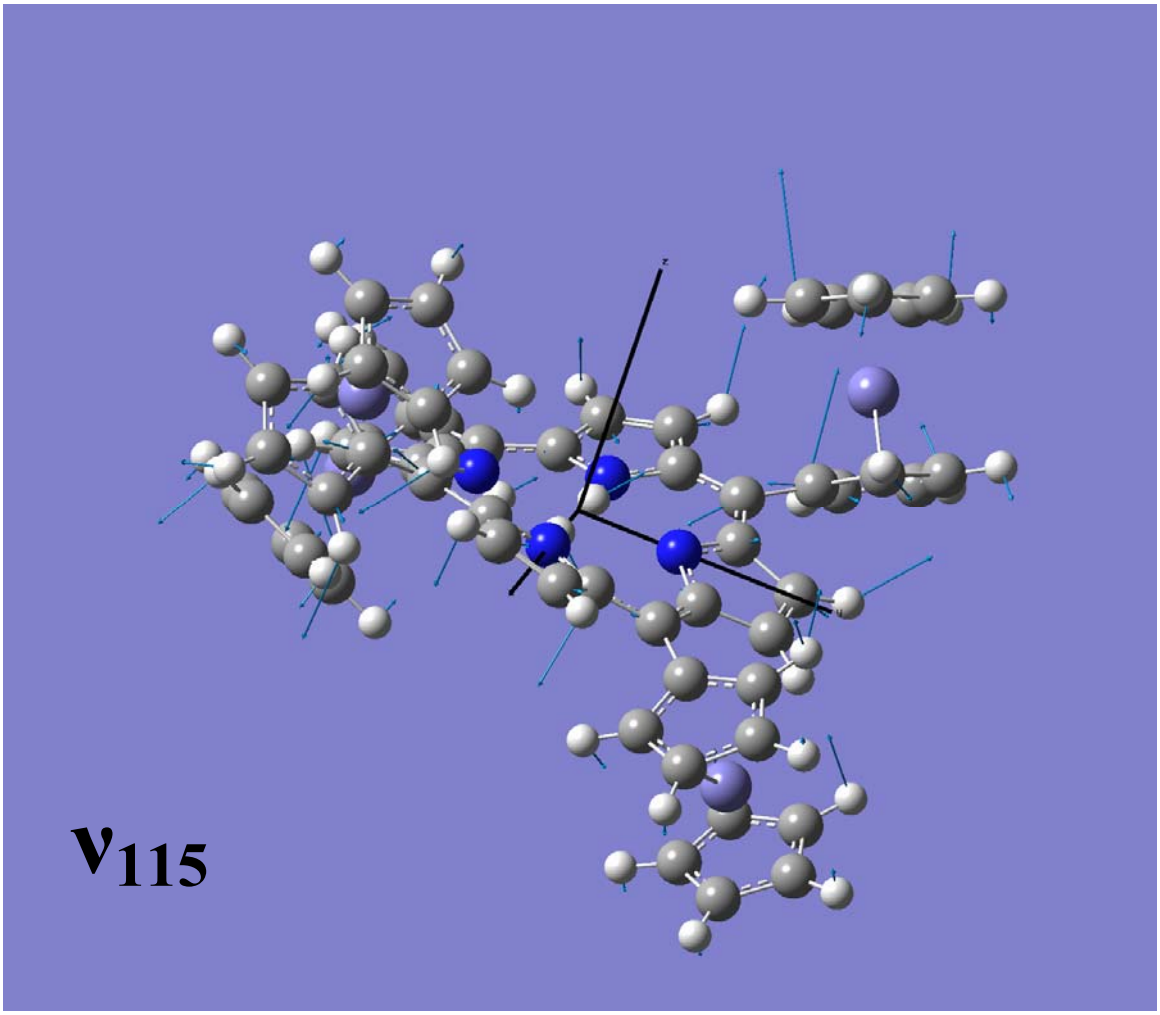

ν113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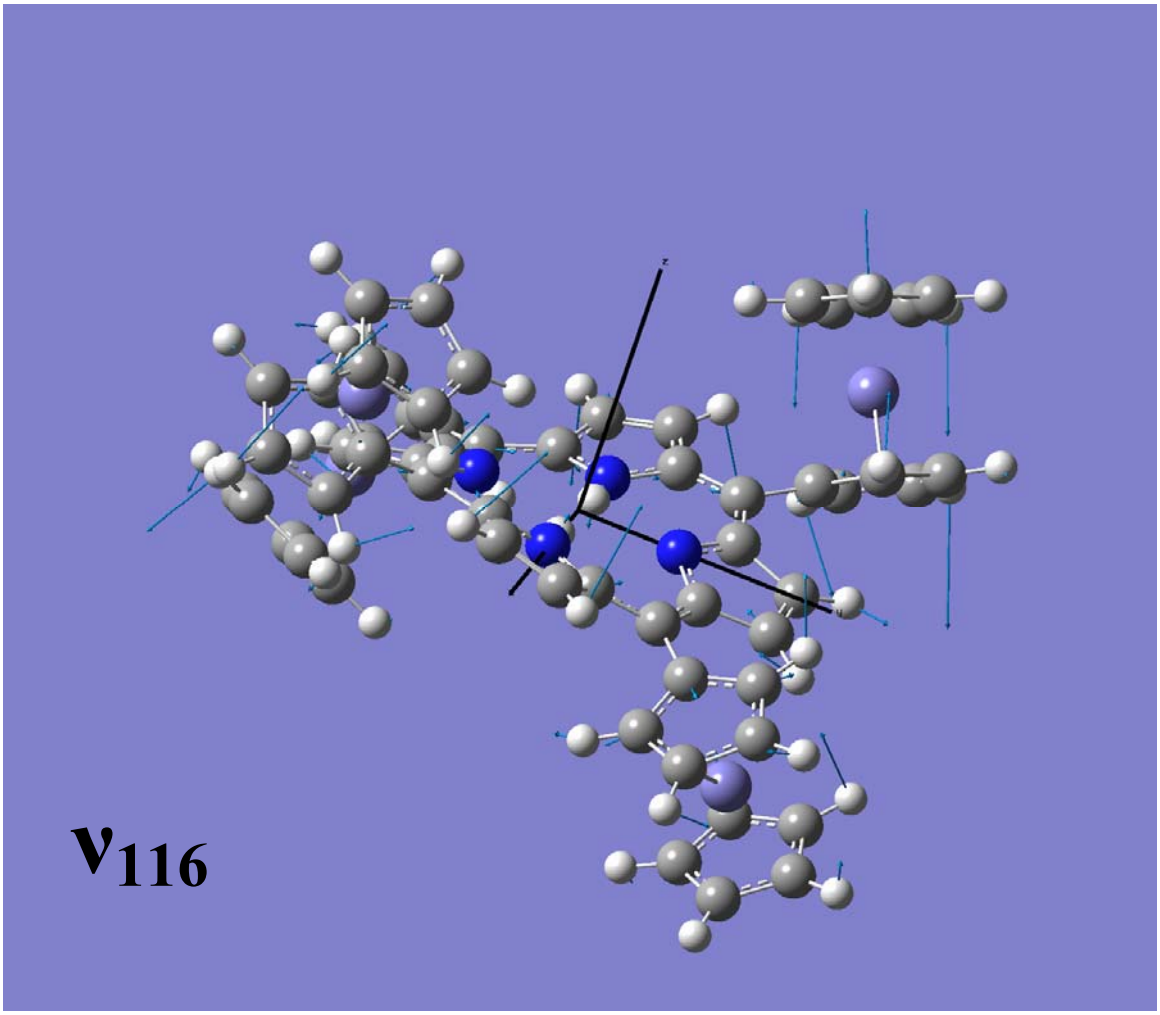
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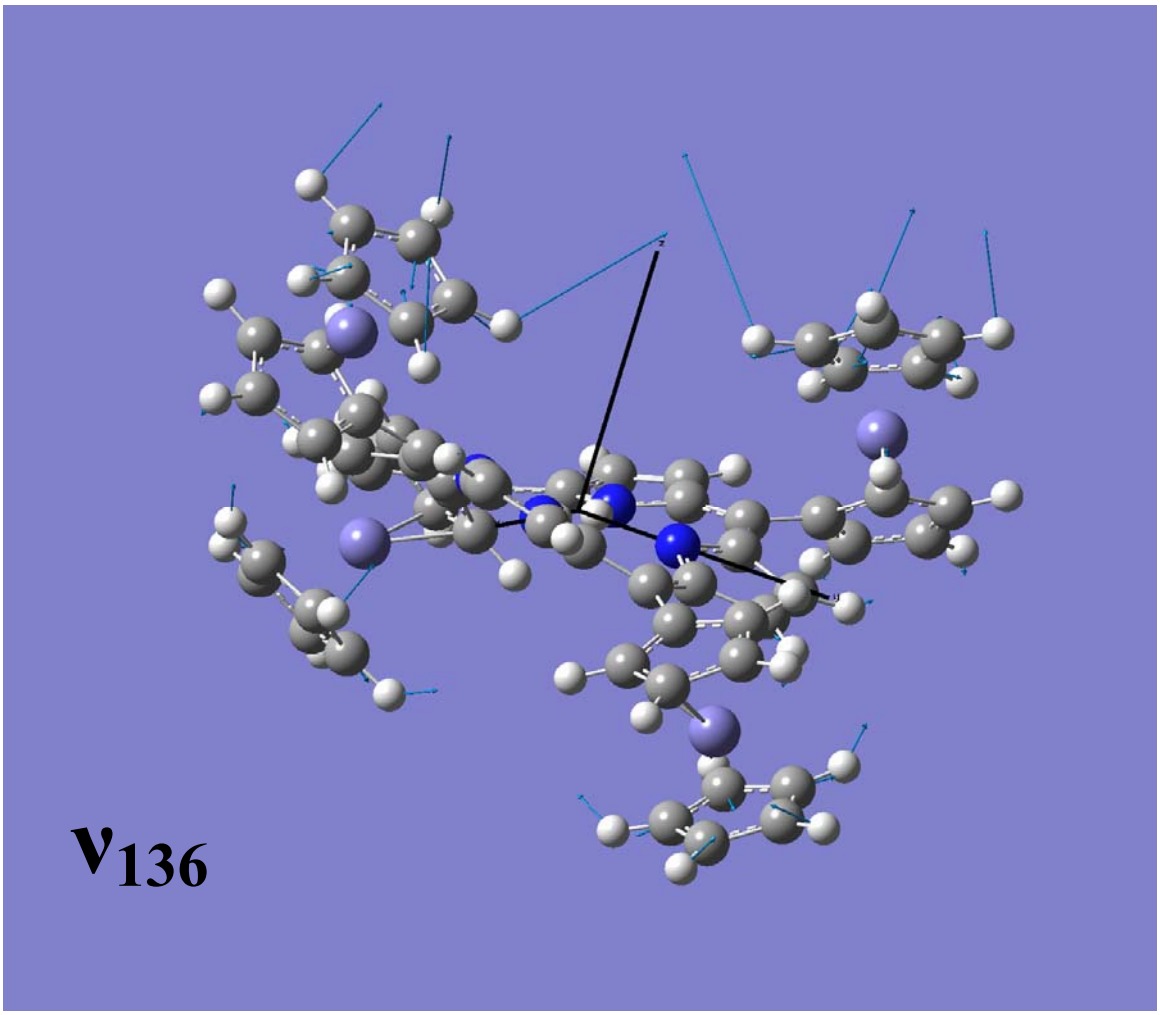
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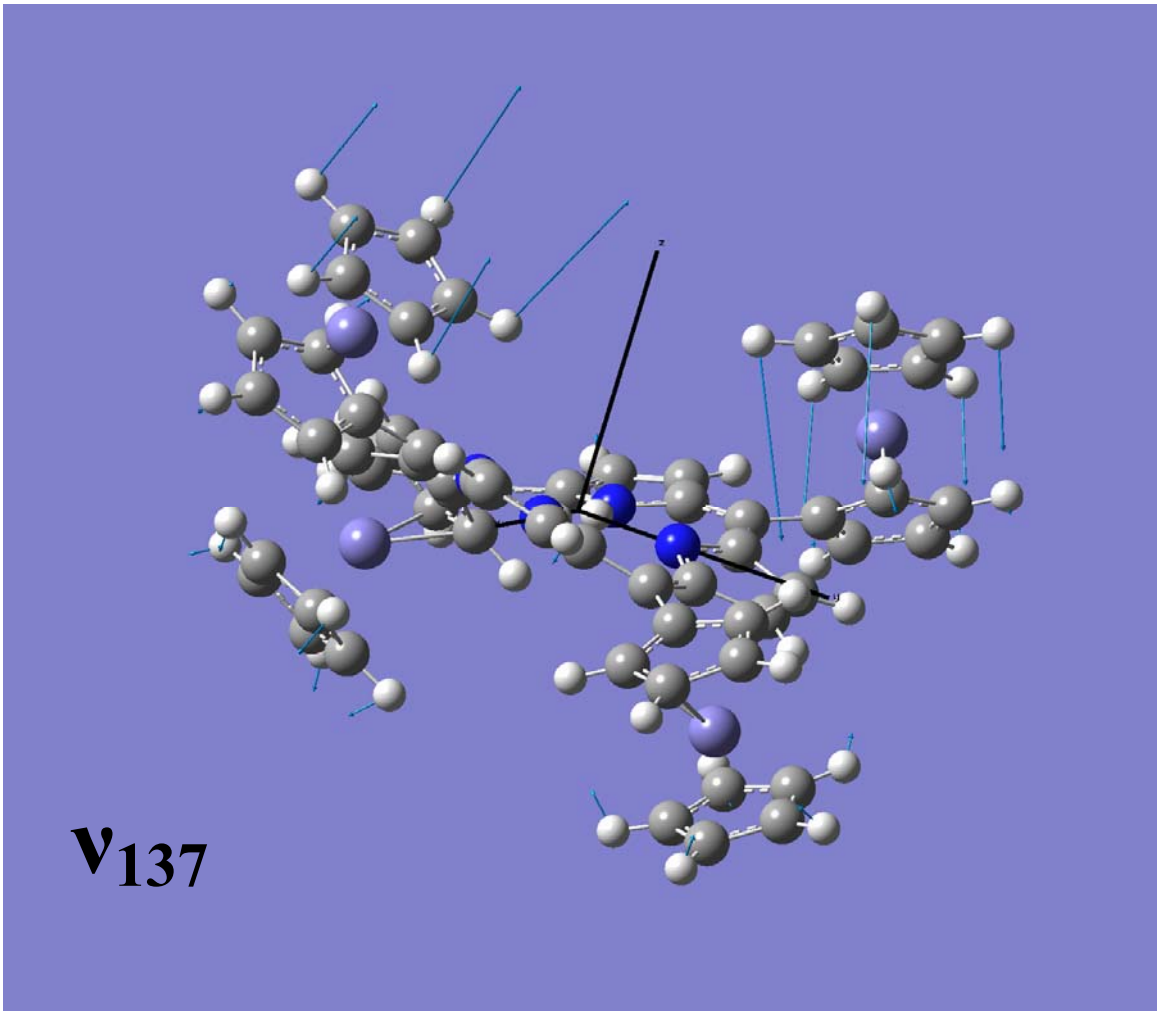
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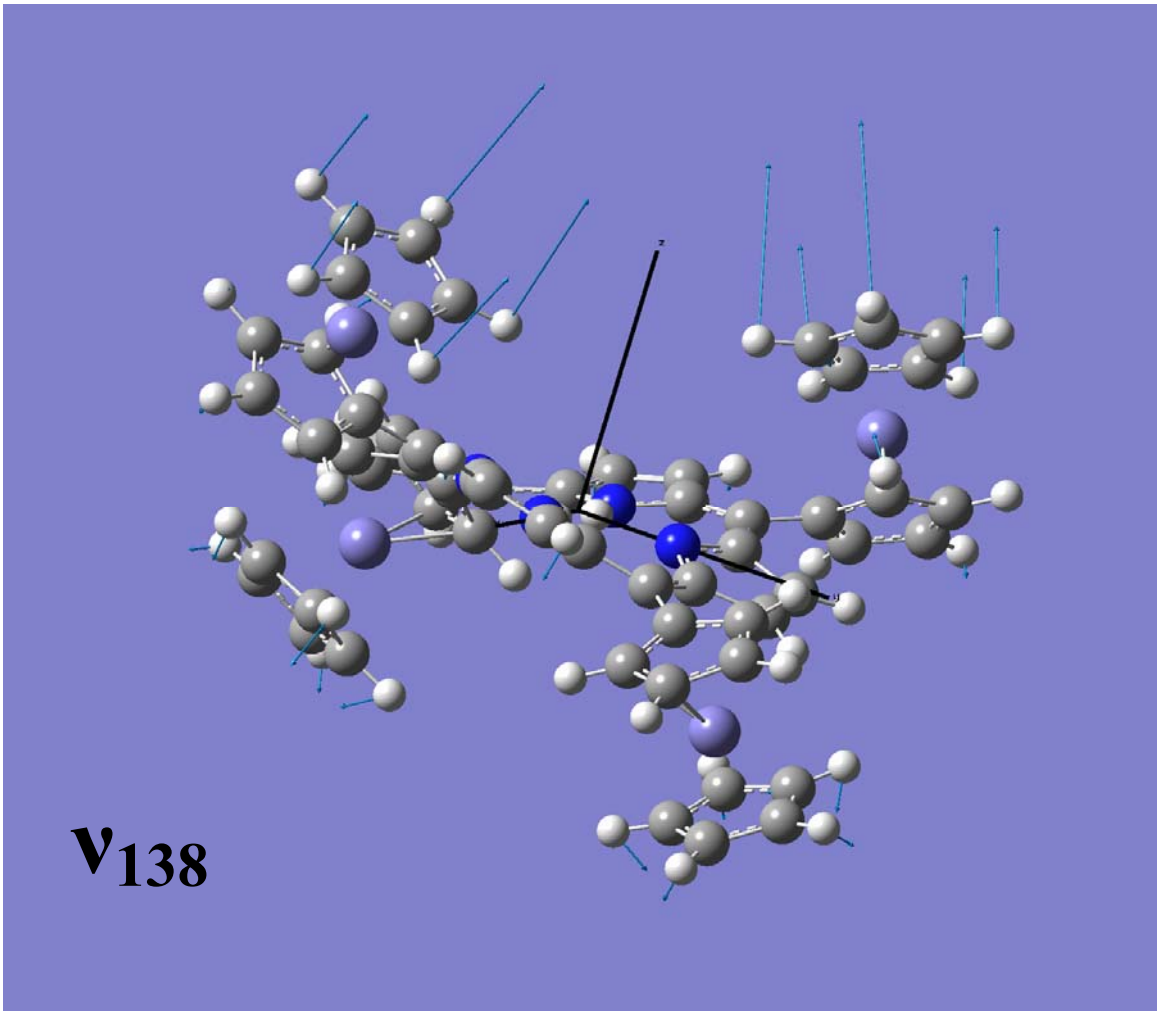
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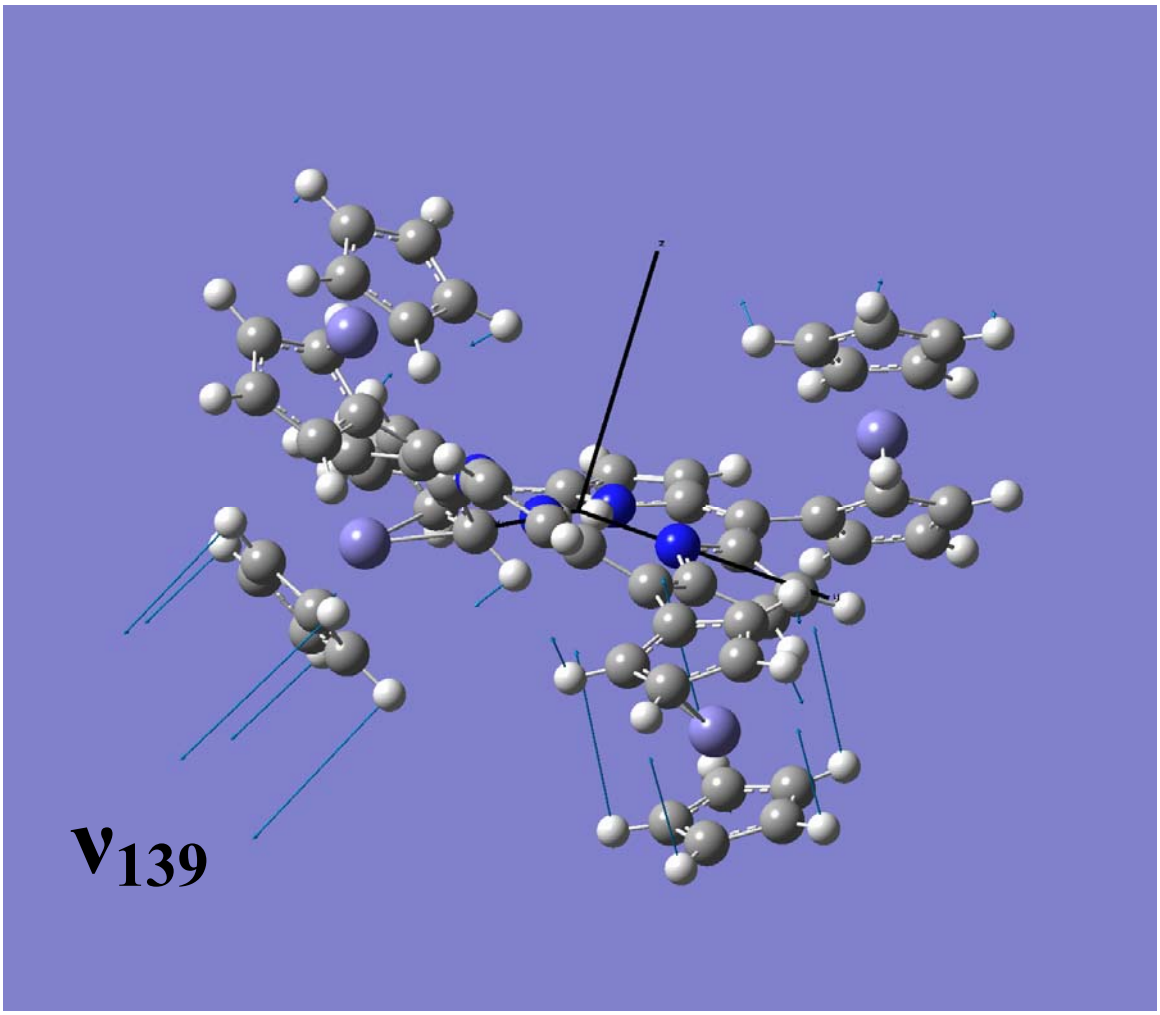
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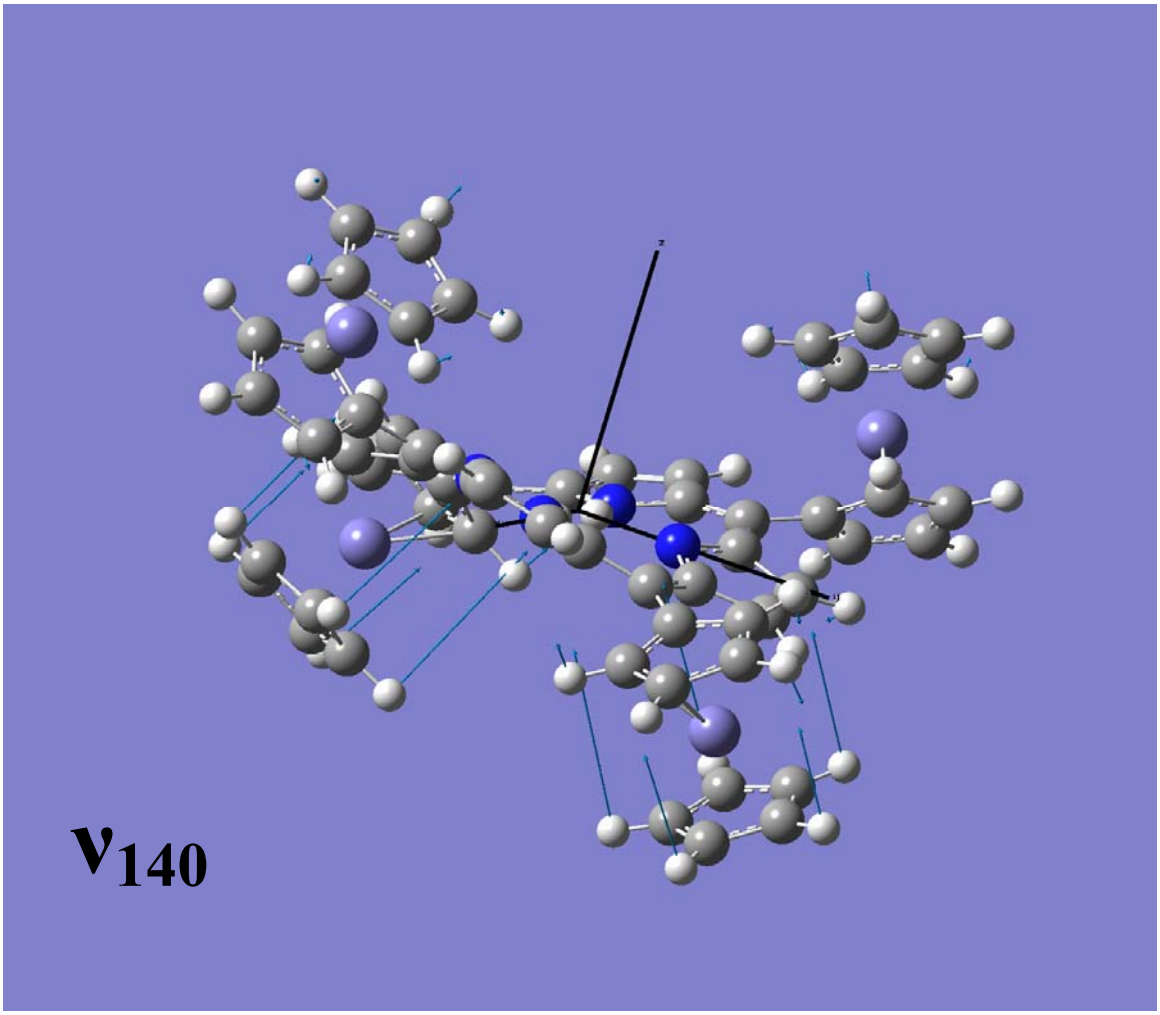
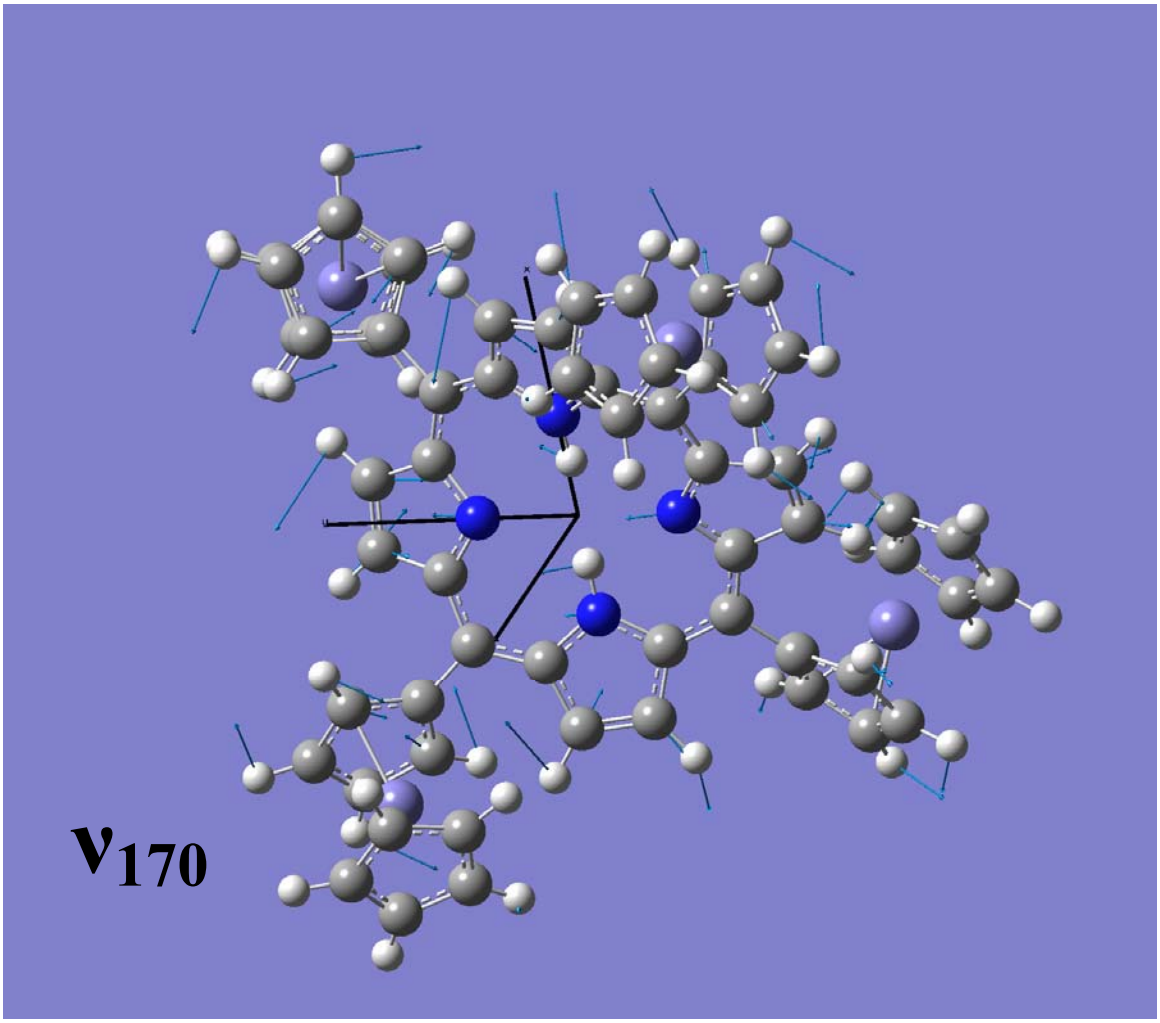

ν140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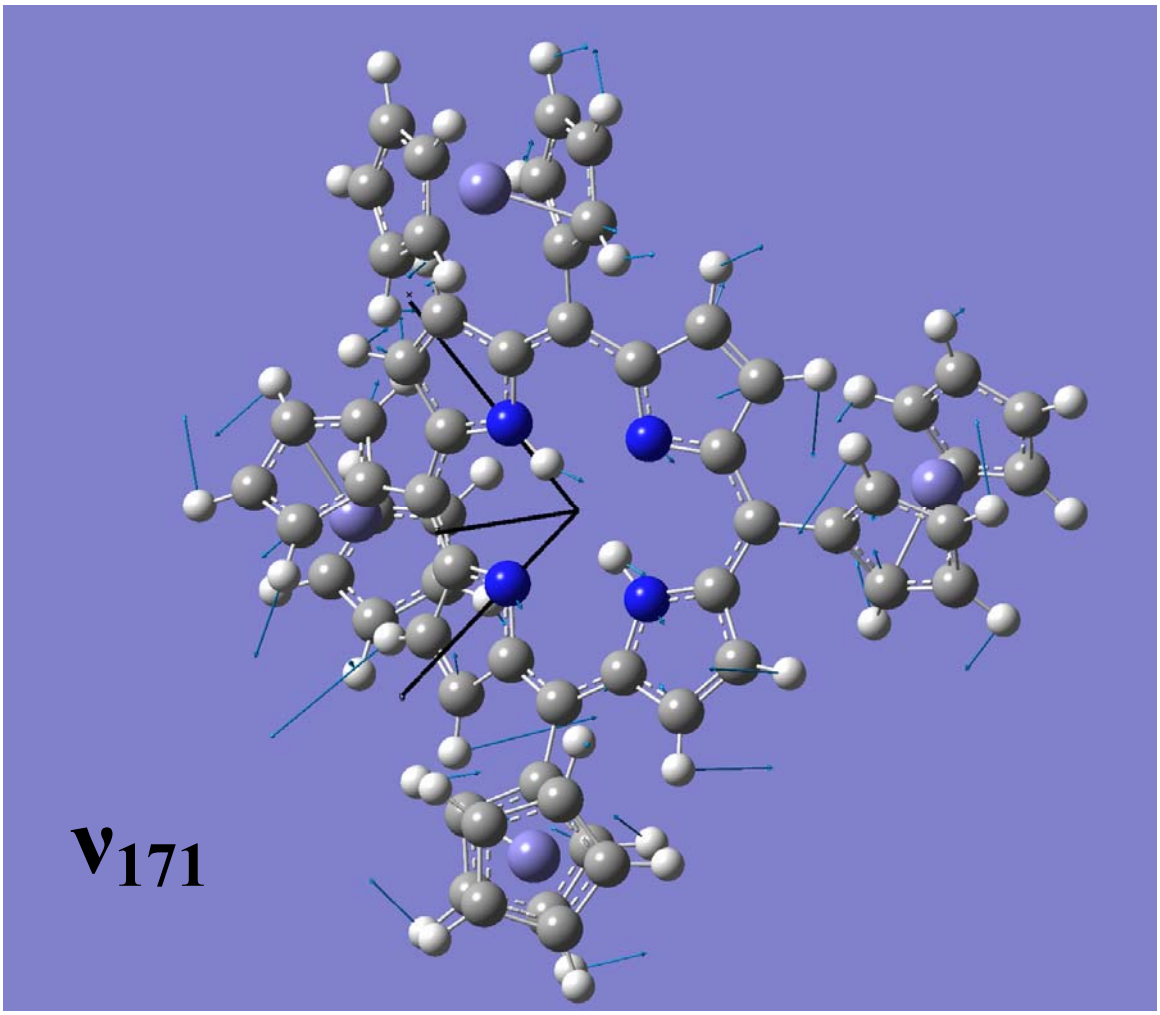
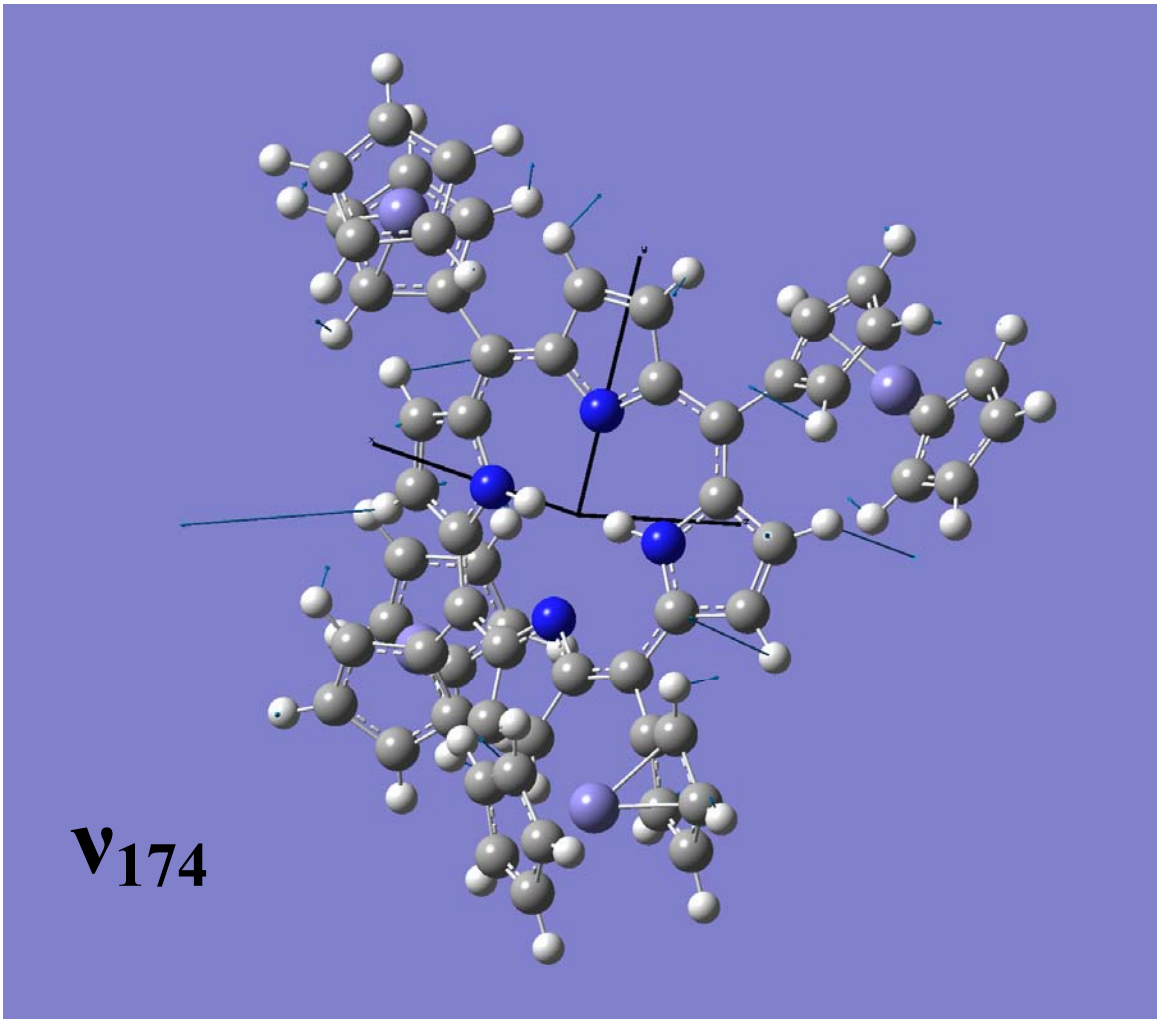

ν_{171}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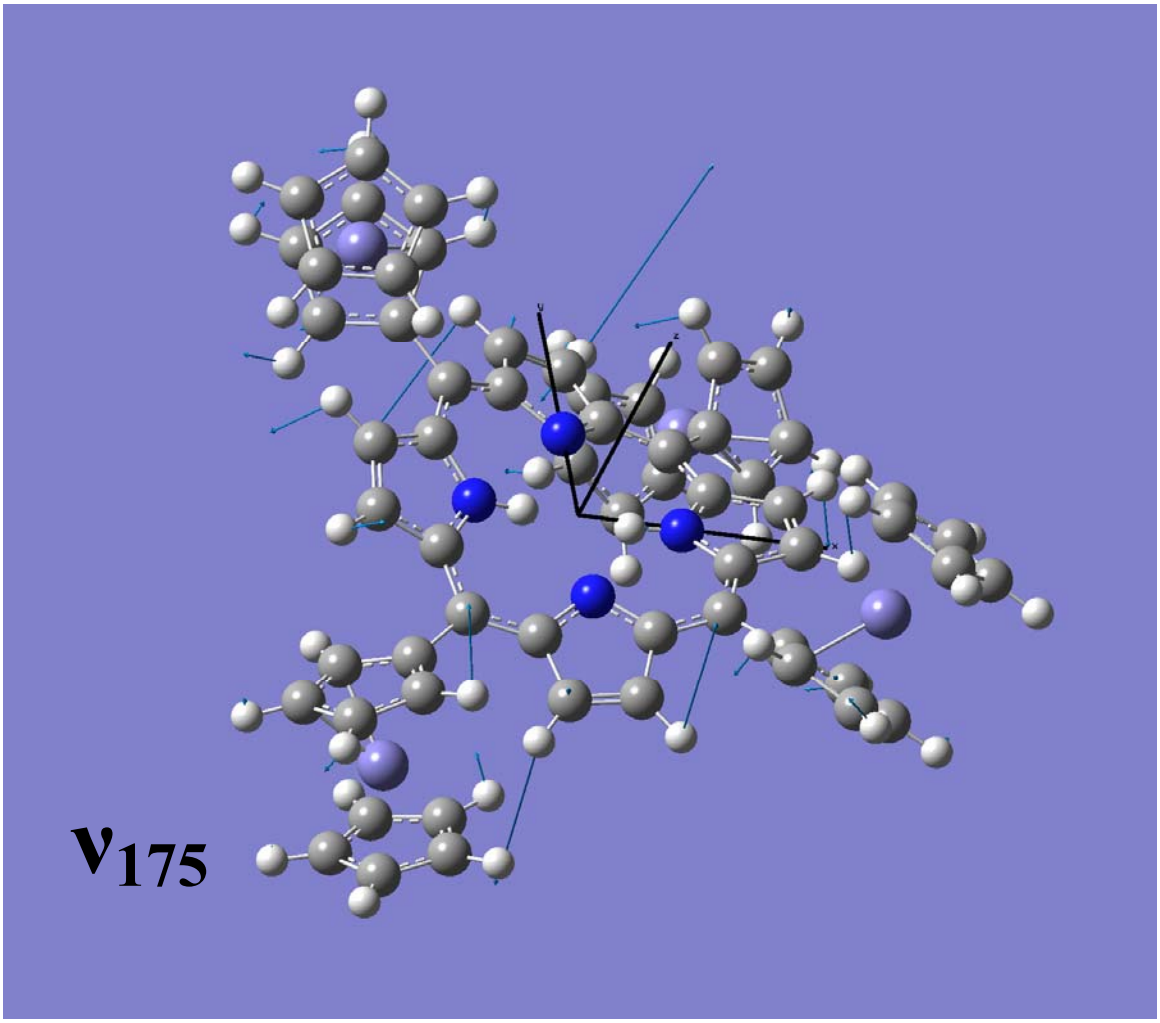
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